1-Nitrobutane

627-05-4 | DTXSID8020967

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 3.01

Global applicability domain: Inside

Local applicability domain index: 9.87e-01

Confidence level: 5.38e-01

Nearest Neighbors from the Training Set

Image not found

Dibromomethane
Measured: 3.07
Predicted: 3.12

Image not found

N,N-Dimethylformamide
Measured: 4.38
Predicted: 3.13

Image not found

n-Hexane
Measured: 2.40
Predicted: 3.19

Image not found

Isopropyl ether
Measured: 2.66
Predicted: 2.82

Image not found

1-Hexene
Measured: 2.41
Predicted: 2.75